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A CRITICAL ASSESSMENT OF MODELS AVAILABLE FOR THE SHOCK INITIATION OF HETEROGENEOUS EXPLOSIVES

(4)

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A CRITICAL ASSESSMENT OF BURN MODELS AVAILABLE FOR IMPLEMENTATION INTO A COMPUTER CODE TO MODEL SHOCK INITIATION OF HETEROGENEOUS EXPLOSIVES

David A. Jones

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ABSTRACT

Several recent models for the shock initiation of heterogeneous explosives are presented, concentrating on those models which have proved to be the most successful. Particular attention is given to models of specific interest to MRL, which are capable of simulating the effect of particle size on sensitivity, and can be readily incorporated into single phase hydrodynamic computer codes. Other models are also briefly considered. Recommendations are made regarding the suitability of some of these models for MRL use.

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A CRITICAL ASSESSMENT OF BURN MODELS AVAILABLE FOR IMPLEMENTATION INTO A COMPUTER CODE TO MODEL SHOCK INITIATION OF HETEROGENEOUS EXPLOSIVES

1. INTRODUCTION

There has been considerable interest for some years at Materials Research Laboratory in the numerical simulation of shock and detonation phenomena in condensed energetic materials. Our early experience in non-reactive shocks involved use of the HELP code, a multimaterial two-dimensional Eulerian code for the numerical simulation of hydrodynamic and elastic-plastic flow. HELP was used primarily for warhead modelling and was particularly useful in the numerical simulation of the MRL 38 mm shaped charge jet [1]. Whilst the general agreement between the code calculations and the flash radiographs was excellent, problems were encountered in calculating an accurate shape for the jet tip because of the numerical scheme used for tracking the interface between the different materials. For these and other reasons, we have now replaced HELP with the HULL code. HULL was originally developed by Systems, Science and Software for the US Air Force and is now maintained by Orlando Technology. The code has both Eulerian and Lagrangian capabilities and can perform simulations in either two or three dimensions. HULL has an extensive library of equation-of-state subroutines for non-reactive media, but only a rudimentary capability for numerical simulation of detonation phenomena.

Modelling the detonation of a condensed explosive at MRL has until now been carried out using the reactive hydrocodes SIN and 2DL developed at Los Alamos National Laboratory by Mader in the 1960s and 1970s [2,3]. Both are one and two-dimensional hydrocodes which were specifically designed to model reactive shock phenomena and they contain a variety of explosive burn subroutines. However, significant advances have been made over the past decade in the understanding of the shock initiation of condensed heterogeneous explosives; SIN and 2DL do not reflect these advances. In particular, the most advanced burn subroutine in 2DL is the Forest Fire model [4], which is an expression for the rate of explosive decomposition as a function of the local pressure which reproduces the observed run-to-detonation distance for a given initial input pressure (the so called Pop plot data) [4]). Forest Fire has proved to be very effective for the numerical simulation of two and three-dimensional reactive shock interactions, but cannot probe the basic physics and chemistry of the shock initiation process. Forest has described a method for estimating changes in the Forest Fire coefficients due to changes in the explosive density [5], but if the explosive particle size is altered (a parameter which has an important influence on the shock initiation behaviour of heterogeneous explosives [6]), then a new series of experiments must be run to generate new Pop plot data for the Forest Fire coefficients. Such experiments are very time consuming and costly, and cannot readily be conducted at MRL.

In the last few years a number of models have been proposed for the shock initiation of heterogeneous explosives which provide some insight into the basic physics

involved. One of the most successful of these is the Ignition and Growth model of Lee and Tarver [7,8]. In this approach the initiation of detonation is divided into two stages: in the first stage the passage of the shock front creates "hot spots", or localized areas of high temperature, at density discontinuities in the heterogeneous explosive. In the second stage these hot spots grow, by a grain burning process, and then eventually coalesce to form a stable detonation. While the Ignition and Growth model has greatly increased our understanding of the shock initiation process, it is still a phenomenological model in the sense that the coefficients, which have to be fitted to experimental embedded gauge data, need to be redetermined each time one of the physical properties of the explosive is changed.

In a recent paper Kim has developed a model which incorporates physical properties of the explosive such as grain size and porosity in a simple and yet effective manner [9]. By focussing attention on the basic physics of the shock initiation process he has been able to develop a version of the Ignition and Growth model which contains fewer adjustable constants than the original, and which has the advantage that once these constants are determined (again, by comparison with pressure-time histories provided by embedded gauge data), they do not have to be changed to accommodate variations in grain size or density/porosity.

The purpose of this report is to examine several recent shock initiation models in detail, and to assess their suitability for implementation in existing hydrocodes at MRL. We begin by first describing several of the mechanisms which have been proposed for the formation of hot spots in heterogeneous explosives. Next, a critical examination of the Ignition and Growth model of Lee and Tarver is made, followed by the model of Kim. A different approach is discussed in section 4, based on a coupled set of rate equations for the various processes involved, and appropriate time constants for each of these processes. In section 5 other models which have been proposed recently are briefly described. The intention here is not to review all models exhaustively, but rather to concentrate on those models of most relevance to our own needs. In the conclusion, the relative merits and disadvantages of these models are discussed and their ease of implementation in various hydrocodes are considered.

2. PROPOSED MECHANISMS FOR HOT SPOT FORMATION

The shock initiation of a heterogeneous explosive differs fundamentally from that of a homogeneous one. The differences were clearly described in the early 1960s in two extensive experimental papers by the Los Alamos group of Campbell, Davis, Ramsay and Travis [6,10]. In a homogeneous explosive, such as a liquid or a single crystal, detonation is caused by a thermal explosion due to the bulk heating of the sample by the passage of the shock.

In a heterogeneous explosive the situation is more complicated. Most condensed explosives consist of polycrystalline materials containing voids of various shapes and sizes, defect structures, and often small amounts of polymeric binders and plasticisers. When a shock wave travels through such material it provides heating both by bulk compression and by the interaction of the shock with the various density discontinuities and defect structures. The localised regions of high temperature caused by these density discontinuities, the hot spots, may then begin to react and, if conditions are favourable, may lead to the formation of a stable detonation even though the temperature rise caused by the bulk heating may be insufficient by itself to lead to detonation [17].

This situation is illustrated by the shock initiation of the explosive PETN [11]. For a single crystal of PETN to detonate within 1 μs it has to be shocked to 11 GPa, which produces a bulk temperature of 570°C. But if the PETN is in powder form and pressed to almost crystal density it requires a shock of only 2.5 GPa. The bulk temperature in this case is only 145°C and would be insufficient to cause detonation within 1 μs.

Current understanding of the initiation of detonation in heterogeneous explosives by shock divides the process into two distinct stages.

(i) Ignition of a small fraction of the explosive at random sites within the sample due to the creation of hot spots.

(ii) Buildup to detonation from the energy released by the grain burning processes growing from the original hot spots. If steady detonation is to be attained it is essential that any losses in energy must be less than the energy released by the hot spots.

There is clear experimental evidence supporting this picture of the initiation process [12]. To numerically simulate shock initiation we therefore need to find appropriate models for both the ignition and buildup stages. Many models of hot spot formation have been proposed for the ignition stage and these are listed below.

1. Stagnation of microjets [13].
2. The hydrodynamic hot spot [14].
3. Visco-plastic heating in material near the surface of a collapsing void [15].
4. Shock collision around high impedance inclusions [16].
5. Friction between crystal grains [17].
6. Internal shear banding and dislocation pile-up [18].
7. Adiabatic gas compression [17].

The buildup stage is usually modelled by a grain burning process as first proposed by Eyring [19]. There is ample experimental evidence for the importance of this mechanism in the buildup stage [20,21], and grain burning models will be discussed in more detail in the following sections. In the remainder of this section a brief description is given of some of the proposed mechanisms for hot spot formation listed above.

The stagnation of microjets theory was first proposed by Seely [13]. The basic idea is that as the propagating shock exits an explosive grain it causes material to fly off the grain surface. As the grains are randomly oriented with respect to one another the material can interact in various ways, and in some cases jets will be produced. Seely assumes that these jets will behave hydrodynamically, and after traversing a typical void space they will collide with the surface directly ahead, and stagnate. Seely uses simple arguments to show that the hot spot temperature produced by this mechanism is proportional to the square of the particle velocity immediately behind the shock front. Lee and Tarver have been able to represent this mechanism in their original ignition and growth model [7], and we will comment on the degree to which it agrees with experiment in the next section.

Mader has proposed a hydrodynamic void closure mechanism to explain hot spot formation [14]. In this model the passage of the shock front causes collapse of the void, and high temperatures are produced by the high impact pressures and focussing effects during the collapse process. Mader has extended this model to three dimensions and shown that it is capable of reproducing the observed desensitization of heterogeneous explosives by a weak preshock [22]. In this case the preshock closes the voids but the hot spots formed do not have high enough temperatures to build up to detonation. The following shock then sees an effectively homogenous material, and is therefore less sensitive to shock initiation.

The visco-plastic heating of the material in a thin shell surrounding the surface of a collapsing void has been considered by several authors [15,23,24]. Frey [15] has presented quite a detailed description of cavity collapse in energetic materials based on earlier work of Carroll and Holt [25]. He has considered hot spot formation due to inviscid plastic work, viscoplastic work, gas phase heating, and solid phase compression (ie. the hydrodynamic model proposed by Mader), and presented a very comprehensive analysis of the conditions under which each mechanism will occur. His main conclusion is that viscoplastic work is by far the most efficient mechanism for producing high temperatures, and is favoured by high viscosity, low yield strength, and short rise times.

Frey was unable to include the formation of shear bands in his model of cavity collapse, but has considered this mechanism in detail elsewhere [26]. Coffey has also studied the effect of shear banding on shock initiation [27, 28]. These authors have shown that significant heating can occur in crystalline explosives by the generation and movement of dislocations and the localization of these dislocations in shear bands in the deforming solid. Direct experimental evidence that shear bands are important in the initiation of explosives can be found in the paper by Field, Swallowe and Heavens [29]. The conditions under which shear banding is the dominant mechanism for hot spot formation in any given situation do not seem to be as well characterised as those mechanisms previously discussed, although it is certainly an important mechanism under impact conditions.

Adiabatic gas compression heating was also considered by Frey [15], and was shown to make a negligible contribution to the temperature increase under typical shock initiation conditions. For impact conditions however adiabatic gas compression can be important.

3. THE IGNITION AND GROWTH MODEL

In their original model Lee and Tarver [7] divided the initiation process into two distinct stages. In the first, the ignition stage, the passage of the shock front creates localised regions of high temperature (the hot spots) at density discontinuities within the heterogeneous material. In the second, the growth (or build up) stage, these hot spots were postulated to grow by a grain burning process until they eventually coalesced to form a stable detonation. The model is phenomenological in the sense that plausable assumptions are made regarding the physical mechanisms for each of these stages and then a generalized energy release rate equation of the form

$$\frac{\partial F}{\partial t} = I(1 - F)^x \eta^r + G(1 - F)^x F^y P^z \qquad (1)$$

$$\eta = \rho_s/\rho_0 - 1 \qquad (2)$$

is considered, where F is the fraction of explosive that has reacted, ρ_0 is the initial density, ρ_s is the density of shocked explosive, P is the pressure, and I, G, x, y, r and z are constants which must be determined experimentally.

Different models of hot spot formation lead to different values for the constant r. In the first reported application of the model the ignition rate was assumed to be proportional to the strain rate in the shocked explosive, which corresponds to a value of r = 1 in equation (1). Some success was achieved in modelling shock initiation experiments in PBX-9404 (HMX/NC/TCP 94:3:3), but this value was later found to be innappropriate over

an extended range of stimuli or material properties [7]. A value of r = 3 corresponds to a hot-spot formation model due to the stagnation of microjets, first described by Seely, [13], while r = 4 describes a model based on the amount of plastic work in the void or cavity walls required for void collapse. Best overall agreement with experiment was found when r = 4 was used in equation (1) [7].

The constants x and y are related to the choice of the geometry for the hot spot combustion process. Hot spots can be considered to burn outward from the void centre, or inward over the total grain surface. Lee and Tarver considered a spherical hot spot burning outward, which corresponds to y = 2/3. Requiring that the rate be a maximum when the combustion surfaces overlap leads to the value x = 2/9.

The remaining constants I, G and z were found by fitting to the detailed shapes of embedded pressure gauge records and run distance to detonation data. Values of these constants for the three pressed explosives PBX-9404, TATB, PETN and cast TNT are shown in Table 1. The P^z term in equation (1) represents a laminar burn rate and the constant G corresponds to a surface area to volume ratio. Measured values of z for laminar deflagration rates in explosives are usually of the order of 0.8 to 1.0 for pressures below 0.1 GPa. The higher values for z reported in Table 1 are probably caused by grain fracture occuring due to the higher pressures generated. Lee and Tarver also used equation (1) with a fixed value for z of 1.0. They found that they could reproduce all the buildup and run distance to detonation data from embedded pressure gauges by allowing the growth coefficient G to increase as the input shock pressure increased.

Equation (1) was combined with the Jones-Wilkins-Lee equation of state both for unreacted explosives and their reaction products and implemented in a one-dimensional Lagrangian hydrodynamic code. Using the values of the constants described above, and shown in Table 1, the model was able to successfully calculate all the sustained pulse manganin pressure gauge and particle velocity data for the four explosives at densities near their theoretical maximum densities. Lee and Tarver also found that these same constants gave a reasonable prediction of the shock initiation properties of the same explosives at lower densities.

The model was also applied to short pulse duration shock initiation experiments [7] and there it was less successful. Detailed quantitative modelling of experimental data was only possible if the coefficient for the growth of reaction was increased by a factor of two or three. To overcome these difficulties Tarver, Hallquist and Erickson proposed a three term ignition and growth model [8]. Their expression for the chemical reaction rate equation is

$$\frac{\partial F}{\partial t} = I(1 - F)^b \left(\frac{\rho}{\rho_0} - 1 - a\right)^x + G_1(1 - F)^c F^d P^y + G_2(1 - F)^e F^g P^z. \qquad (3)$$

The parameter a is used to prohibit ignition until a certain degree of compression has been reached. Values for the constants I, G_1, G_2, a, b, c, d, e, g, x, y and z for the explosives PBX-9404 and LX-17 (TATB/KelF800 92.5:7.5) are given in Table 2.

The main idea behind the three term reaction rate model is to split the growth term into two parts. The first part models the relatively slow pressure and particle velocity increases behind the shock front in the early stages of hot-spot growth, and consequently the constant y has the value 1.0 to correspond to measured values in deflagration experiments. The second part of the growth term describes the rapid completion of the reaction as the hot-spots begin to coalesce. With G_1 and G_2 fixed, the

value of z is therefore greater than 1.0. Equation (3) was used with the parameters given in Table 2 and yielded good overall agreement with a large collection of shock initiation data on PBX-9404 from three laboratories [8].

While the ignition and growth model has successfully calculated a great deal of one and two-dimensional experimental data on heterogeneous explosives it is still a phenomenological model in the sense that it does not attempt to model in detail the processes that cause the heterogeneous heating of the explosive. Consequently it is not capable of modelling the effect of particle size or initial temperature on shock initiation. Cochran and Tarver overcame this problem by developing a statistical treatment of hot-spot formation which does take these physical parameters into account and which can be used with the ignition and growth model [30]. They have applied this combined model to LX-17 and have been able to successfully reproduce experimental manganin pressure gauge records for different particle sizes, as well as Pop plots determined at different initial temperatures.

4. THE KIM MODEL

Kim has recently described an ignition and growth model which incorporates particle size effects in a natural manner [9]. The model is based on previous work by Carroll and Holt [25], who showed that a simple hollow sphere model was effective in describing the compaction process in powdered materials. In the Kim model the hot-spots are assumed to be generated around pores (voids) in the compacted explosive. As we have noted in Section 2, there are many physical mechanisms which can lead to hot-spot generation in shocked porous explosives. Kim and Sohn [23] have pointed out that, apart from adiabatic gas compression (which does not contribute significantly at the high pressures short duration shocks typical of shock initiation), each of these mechanisms is simply one form or another of mechanical deformation of the explosive crystals, and in a real explosive it is likely that several of these mechanisms may be operating simultaneously.

Faced with the impossibility of describing each of these mechanisms in detail, Kim and Sohn [23] adopt a model which is capable of predicting the global behaviour of the deforming region. A simple linear elastic-viscoplastic relationship is assumed for the material behaviour:

$$\frac{d\epsilon}{dt} = \gamma_1(\sigma - \sigma_0) + \frac{1}{E}\frac{d\sigma}{dt} \qquad (4)$$

where ϵ is the strain, σ the stress, and σ_0 the static yield strength of the material. The first term on the right hand side of equation (4) describes the viscoplastic response, with γ_1 being the coefficient of viscosity. The second term represents the elastic response, and E is the Young's modulus of the material.

The model adopted for the compaction process assumes that pores within the explosive are uniform in size and distribution. Figure 1 illustrates how a typical void in a porous explosive is represented in the hollow sphere model. If the average particle diameter d_p has a value of 200 μm, then the radius of the outer sphere r_o (also shown as a dotted line in Fig. 1a) is chosen to be 100 μm. If the explosive has a porosity of 2% then the value of the inner radius is determined by requiring that the ratio of the volume of the inner sphere to that of the outer sphere should be 0.02, leading to a value for r_i of $(0.02)^{1/3}$ r_o. The equations of motion for the compression of the material surrounding the pore have the form

$$\frac{\partial \sigma_r}{\partial r} + 2\,\frac{(\sigma_r - \sigma_\theta)}{r} = 0 \tag{5}$$

$$\frac{\partial v}{\partial r} - \frac{v}{r} = \sqrt{3}\gamma\left(\frac{(\sigma_r - \sigma_\theta)}{\sqrt{3}\,k} - 1\right) + \frac{1}{2G}\,\frac{\partial}{\partial t}\,(\sigma_r - \sigma_\theta) \tag{6}$$

$$\frac{\partial v}{\partial r} + 2\,\frac{v}{r} = 0 \tag{7}$$

where σ_r is the radial stress, σ_θ is the tangential stress, r is the space coordinate, v is the radial displacement rate,

$$\gamma = \gamma_1 \sigma_0,\ k = \sigma_0/\sqrt{3},\ \text{and}\ G = E/3.$$

These can be solved analytically using Laplace transforms, and an expression for the temperature rise within the material due to bulk mechanical deformation can be written as follows:

$$\frac{dT}{dt} = \left(\frac{q}{4\rho C_p}\right) \frac{\left(P_0 - P_g - 2\sqrt{3}\,k \ell n \dfrac{r_o}{r_i}\right)^2}{\left(r_i^{-3} - r_0^{-3}\right)^2 r^6} \cdot \frac{\gamma_1}{\sqrt{3}} \tag{8}$$

Here ρ is the solid density, C_p its heat capacity, P_0 is the applied stress at r_0 and P_g is the gas pressure in the void. The temperature rise within the explosive due to this mechanical deformation leads to both heat conduction and chemical reaction. The equation describing the overall temperature change can therefore be written as

$$\rho\, C_p\, \frac{\partial T(r,t)}{\partial t} = \rho\, C_p\, \left(\frac{\partial T}{\partial t}\right) + \frac{1}{r^2}\,\frac{\partial}{\partial r}\left(r^2\, k^*\, \frac{\partial T}{\partial r}\right) + Q\,\frac{\partial\, \lambda\,(r,t)}{\partial t} \tag{9}$$

where k^* is the thermal conductivity, Q is the heat of reaction, and λ is the degree of reaction of the explosive, with $\lambda = 1$ when the explosive is fully reacted. The last term in equation (9) is taken to have a simple Arrhenius reaction rate

$$\frac{\partial \lambda(r,t)}{\partial t} = (1 - \lambda)\, Z \exp\left\{ - \frac{T^*}{T(r,t)} \right\} \tag{10}$$

where Z is the frequency factor and T^* is the activation temperature.

The model under discussion here is a microscopic model in the sense that $\lambda(r,t)$ represents a local reaction rate within the shell of material surrounding the hollow sphere, showing a maximum at the inner radius r_i and a minimum at the outer radius r_o, and a monotonic decrease between. Use of this expression in a macroscopic hydrodynamic code requires it to be first averaged over the microscopic coordinate r. The local reaction rate is hence integrated over the material within the shell to define a macroscopic reaction rate as follows

$$\lambda(t)_{ign} = \int_{r_i}^{r_o} \lambda\,(r,t)\; 4\pi r^2\, dr \;/\; \frac{4}{3}\,(r_o^{\,3} - r_i^{\,3}). \qquad (11)$$

We now consider the terms used to describe the growth of the reaction after ignition by the mechanical deformation described above. In the early stages of chemical reaction it is assumed that the reaction progresses outward from the surface of the hollow sphere in a surface burning mode. The reaction rate can therefore be expressed as

$$\frac{d\lambda}{dt} = \frac{AP^y\,\lambda^{2/3}}{r_o} \qquad (12)$$

where A and y are constants which describe the slow burning rate at the low pressures found at the beginning stage of the reaction. After the reaction has progressed to a significant degree the burning will have penetrated all the crevices between the particles and the reaction will then be dominated by inward burning of the individual particles. This change in geometry results in a reaction rate of the form

$$\frac{d\lambda}{dt} = \frac{BP^z\,(1-\lambda)^{2/3}}{r_o} \qquad (13)$$

where now the constants B and z describe the fast burning rate at the high pressures generated near the completion of the reaction.

Only five coefficients need to be fitted to experimental data to describe the shock initiation of a porous explosive using this model. These are the constants A, B, y, z, and the material viscosity parameter γ_1 (the constant E was found to have no effect on the results and is no longer considered); all other constants are known. Kim has applied the model to shock initiation data for PBX-9404 and found good agreement with pressure-time histories obtained from embedded stress gauges. He has also considered an imaginary explosive with a particle size four times smaller than in the PBX-9404 study and explicitly shown that the explosive with the smaller particle size is harder to initiate, but transits to detonation more readily, than the explosive with the larger particle size. This behaviour is in agreement with known experimental results [46]. Calculations are currently underway to model particle size effects in the explosive HNS [31].

5. THE EMPIRICAL HOT SPOT MODEL

The empirical hot spot model has been developed in a series of papers by Johnson, Tang and Forest of Los Alamos National Laboratory [32-36]. Unlike the approach of Kim, and to a lesser extent that of Lee and Tarver, no attempt is made to explicitly model any of the physical mechanisms leading to hot-spot formation. Instead, time constants are defined for each of the significant processes involved in the overall shock-to-detonation transition, and a series of rate equations written down which govern the time dependence of each of these processes. This is achieved using the following approach.

Let τ_s represent the characteristic time for hot spot excitation due to the passage of the shock front. The decomposition of these hot spots is then characterized by the time constant τ_c. The process for the transport of energy from the hot products of

the hot spot decomposition to the colder bulk explosive is then governed by the characteristic time τ_m. Finally, τ_d is the characteristic time for decomposition in the bulk explosive once the transfer of energy from the hot spots has taken place. A set of six coupled rate equations can then be written down to describe the time dependence of the reactants, intermediates, and products, for both hot spots and the remainder of the explosive. This constitutes a very general model for the overall shock-to-detonation transition.

By making some plausable physical assumptions Tang, Johnson and Forest [33] are able to considerably simplify the general model. They assume that the shock process which leads to the formation of the hot spots will be very much faster than the process leading to their decomposition, ie. they make the approximation

$$\tau_c >> \tau_s \tag{14}$$

Also, they assume that the energy transfer process from the hot products of the hot-spot decomposition to the balance of the explosive will be much slower than the decomposition of the remainder of the explosive, ie. they make the approximation

$$\tau_m >> \tau_d \tag{15}$$

With the use of conditions (14) and (15) the six coupled rate equations reduce to just two coupled equations, these being

$$\frac{d\lambda_h}{dt} = \frac{1}{\tau_c} (1 - \lambda_h) \tag{16}$$

and

$$\frac{d\lambda_b}{dt} = \frac{\mu}{\tau_m} (1 - \lambda_b) \left(\frac{\lambda_h - f_0}{1 - f_0}\right) \tag{17}$$

where μ is the hot spot mass fraction, f_0 is a threshold value of the normalized mass fraction of hot spot reaction that must be reached before the burn can propagate into the explosive, λ_h is the mass fraction of hot spot products divided by μ, and λ_b is the mass fraction of the products of the balance of the explosive divided by $(1 - \mu)$. The overall reaction rate variable λ is given by

$$\lambda = \mu\lambda_h + (1 - \mu) \lambda_b, \tag{18}$$

and its rate of change governed by the equation

$$\frac{d\lambda}{dt} = \frac{\mu}{\tau_c} (1 - \lambda_h) + \frac{\mu}{\tau_m} [(1 - \lambda) - \mu (1 - \lambda_h)] \left(\frac{\lambda_h - f_0}{1 - f_0}\right) \tag{19}$$

Use of equations (16) and (19) requires that expressions must be found for the characteristic times τ_c and τ_m. In the empirical hot-spot model it is assumed that the passage of the initial shock wave of pressure amplitude P_s produces an average hot-spot

temperature T_s given by

$$T_s = T_0 \left[1 - m \frac{T_0}{T^*} \ell n \left(\frac{P_s}{P_0}\right)\right]^{-1}, \tag{20}$$

where m, T_0 and P_0 are constants and T^* is the Arrhenius activation temperature. The characteristic time τ_c is then identified with the induction time for thermal explosion of the hot spot, given by

$$\tau_c = \frac{T_s^2}{T^* \beta Z} \exp\left(\frac{T^*}{T_s}\right), \tag{21}$$

where β is the temperature coefficient due to chemical reaction and Z is the frequency factor for Arrhenius reaction.

The time τ_m characterizes the energy transfer from the hot-spot products to the bulk of the unburned explosive. At low pressures it is assumed that this process will occur by normal heat conduction, while at higher pressures it is expected that both convection and turbulence could become important. The expression for τ_m is therefore composed of two parts:

$$\tau_m = [G_0 P + G(P)]^{-1}. \tag{22}$$

The linear term represents the weaker energy transfer mechanism while G(P) represents the mechanism dominant at higher pressures. Tang, Johnson and Forest [34] in fact show that G(P) should be identified with the Forest Fire rate, and so has the form

$$G(P) = \exp\left(\sum_{i=0}^{n} a_i P^i\right). \tag{23}$$

The empirical hot-spot model, defined by equations (16) and (19-23), has been applied to the explosive PBX-9404 and calibrated to time-resolved particle-velocity data for sustained shocks [32]. A one-dimensional reactive characteristics code was used for the calibration, and the model was able to successfully reproduce all available particle-velocity and Pop plot data. The same model was then used (with identical rate parameters) to simulate the effect of a finite-duration pulse in PBX-9404 [33], and good agreement with experiment was again found. The model has also been implemented in the two-dimensional hydrodynamic finite-element code DYNA2D and used to investigate the two-dimensional effects of corner turning and shock desensitization in PBX-9502 (TATB/Kel-F800 95:5) and again the results have agreed well with experiment [33].

In a more recent application of the model Tang et al [34] have shown that it is capable of reproducing the effect of changes in both density and grain size. Arguments were presented to show that initiation behaviour at lower density could be simulated by increasing the value of the hot-spot mass fraction μ and the reference temperature T_0. Excellent agreement with experimental Pop plot data for PBX-9404 at two different densities was obtained using this approach. The effect of a change in grain size on the fundamental parameters of the theory is more subtle. Tang et al argue that decreasing grain size should lead to an increase in both the sensitivity parameter m and the hot-spot mass fraction μ, but decrease in the hot-spot reference temperature T_0. Changing these constants in the directions indicated does lead to excellent agreement between experiment and simulation for Pop plot data on superfine and micronized TATB. Tang has also used the

model to simulate grain size effects on the performance of boosters [35], and extended the model to include a slow process occuring near the end of the reaction [36].

6. OTHER MODELS

In this section we discuss other approaches to the shock initiation of heterogeneous explosives which have been described recently. A straight forward approach to the determination of the reaction rate law in energetic materials has been described by Anderson et al [37]. This method is based on a Lagrangian analysis of experimental data obtained from embedded manganin pressure gauges. The rate law found using this empirical approach has come to be known as the DAGMAR model (for Direct Analysis Generated Modified Arrhenius Rate). It has the form

$$\frac{d\lambda}{dt} = (1 - \lambda)\, Z_0\, P_s^{\,n} \exp\,(-T^*/_T) \qquad (24)$$

where λ is the fraction of material reacted, P_s the shock strength, T is the temperature, and Z_0, n, and T^* are constants. Equation (24) has been found to provide a good description of the initiation behaviour of PBX-9404 [38] and porous TATB [37]. Note that the pressure term appearing in equation (24) is the initial shock strength, rather than the current pressure P. Anderson et al found inclusion of a shock strength term was crucial for accurate simulation of short-shock experiments. While equation (24) is a useful description of the rate law for the explosives mentioned, it does not describe grain size effects, nor the mechanism by which the hot spots are initially created.

Another expression for the reaction rate law which includes a dependence on the shock strength has been described by Damamme and Missonier [39] and is known as the Krakatoa model. It has the form

$$\frac{d\lambda}{dt} = (N_0)^{1/3}\, K(P)\, H(\lambda), \qquad (25)$$

where N_0 is the number of hot spots per unit volume, K is the radial speed of growth of the decomposing explosive zone, and H is a function which depends on the shape of the hot spots. The model uses the following functional forms:

$$(N_0)^{1/3} = A_m \exp\,(I/I_a) \qquad (26)$$

where I is a function which depends on the shock strength, and A_m and I_a are constants.

$$K(P) = P^n \qquad (27)$$

and

$$H(\lambda) = (1 - \lambda)\,[\ell n\,(1 - \lambda)]^{2/3}. \qquad (28)$$

The Krakatoa model has been applied to a TATB based composition and by suitable choice of the constants A, I_a and n has been able to successfully reproduce experimental Pop plot data.

All the models for shock initiation of heterogeneous explosives discussed so far have been essentially single fluid models, i.e. the reacting material has been treated as a mixture of two coexisting phases; a solid phase consisting of unburned explosive, and a gaseous phase consisting of reaction products. A single reaction variable describes the amount of each phase present, and then the specific volume and energy is defined as a weighted sum of these variables in the separate phases. A suitable equation of state is used for each phase and then pressure and temperature equilibrium between the two phases is assumed. Kip et al have adopted quite a different approach [40]. They have developed a model based on the continuum theory of chemically reacting, multiphase mixtures, and applied it to the heterogeneous explosive PBX-9404. Their model for this particular explosive consists of three phases: phase one is the HMX granules, phase two the nitrocellulose binder, and phase three the reaction products. The TCP is simply treated as an inert additive. Each phase has its own pressure, density, temperature and entropy, and the volume fractions ϕ_i of each phase are treated as independent variables. Separate equations for conservation of mass, momentum and energy are solved for each phase, and various functions C_i^+ describing mass and energy transfer between phases must be defined. In the application to PBX-9404 it is assumed that the hot-spots form in the binder, which is assumed to break down according to Arrhenius kinetics, ie.

$$C_2^+ = - Z_2 \phi_2 \kappa_2 \exp (- T^*/T_2), \tag{29}$$

where κ_2 is the binder density, Z_2 is the frequency factor, and T^* the activation temperature. The HMX particles decompose according to a grain burning model, and so the mass transfer rate for this phase is given by

$$C_1^+ = - W_1(\phi_3^{2/3}/r^0) \phi_1 \kappa_1 P_3^n, \tag{30}$$

where r^0 is the average particle radius, W_1 is the burn velocity, and the pressure exponent n is taken to be a function of the temperature of the HMX particles. This model was implemented in a one-dimensional Lagrangian finite difference code and numerical predictions were compared with a substantial collection of shock and ramp-wave data. Good overall agreement between the simulations and experimental results was found. It should be noted here that the multiphase model for PBX-9404 just described is somewhat atypical in that most explosives do not have an energetic binder such as nitrocellulose.

Baer and Nunziato [41] have also used a two-phase model similar to the one just described to model the deflagration-to-detonation transition in one dimensional columns of HMX. Khasainov et al [24] have also used a two-phase model to simulate the shock initiation behaviour of porous PETN. Hot-spot formulation is modelled by visco-plastic heating around individual pores, and growth of the reaction occurs by surface grain burning. The properties of the solid and gaseous phases are quite different, and are modelled using a two-phase flow theory. Apart from the two-phase formulation, this is similar in some ways to the model described by Kim [9]. The recent work of Nutt [42] is also relevant here as well. He has also modelled hot-spot formation by viscous heating around pore collapse, and has incorporated this with the original growth model of Lee and Tarver [7], and a detailed thermodynamic analysis of a two component reactive system.

7. DISCUSSION

MRL interest in shock initiation is currently centered on surface area effects in the porous explosive HNS for use in slapper detonators, and particle size effects in RDX for use in PBXs and booster explosives. Whichever model is adopted to describe these effects must be capable of implementation in an existing hydrocode at MRL. As previously discussed, only the reactive hydrocodes SIN and 2DL have been used to model the behaviour of explosives. Both are single phase codes which model both the solid phase reactants and gas phase products using the HOM equation of state [4]. More advanced hydrocodes are being developed for reactive flow based on the Flux Corrected Transport technique [44,47], but initial developments will result in single phase codes. Because of this limitation, shock initiation models which can be implemented in single phase codes are of particular interest.

The critical assessment detailed in previous sections has shown that there currently exist a variety of different models of varying degrees of sophistication for the numerical simulation of shock initiation of energetic materials. Because it is virtually impossible, with the current level of understanding, to clearly identify which of the many possible mechanisms will be operable in the ignition and growth processes in a given explosive and or mode of initiation, each model requires a number of adjustable constants. The values for each of these constants are found by fitting to experimental dynamic data, usually pressure-time plots or particle velocity-time plots at specific stations within the explosive. This is an iterative, time consuming process, and so most models have been fitted to only a few explosives.

The Ignition and Growth model [7,8] has probably been fitted to more explosives than any other model. However, it probably also requires the determination of more adjustable constants than any other model. For example, the three term version described by Tarver, Hallquist and Erickson requires the specification of twelve constants [8], and more would be required if particle size effects were to be modelled using the approach of Cochran and Tarver [30].

The Kim model is similar to the Ignition and Growth model but contains a more effective formulation of both the ignition and growth terms, and consequently requires specification of only five adjustable constants. It is, however, more computationally intensive than the Ignition and Growth model as the heat equation has to be solved within each hydrodynamic cell for each time step.

The Empirical Hot Spot model has been extensively developed and successfully applied by its originators to a range of explosives and experimental situations [32-36]. It has successfully modelled both grain size and density effects [34], but its application in this area is not straightforward. Subtle arguements are needed to indicate in which direction various parameters should be changed, and fine tuning of the parameter values is required to fit the experimental results.

The multiphase models have also been extensively developed and applied to a variety of explosives [24,40,41,42,]. These models are considerably more detailed than the single phase models just described, and consequently are capable of providing a better description of the various processes occurring during shock initiation. They also require specification of many more physical parameters, and for this reason are susceptible to problems of non-uniqueness [45]. The numerical coding for multiphase models is also considerably more complicated than for the single phase models.

Because of MRL interest in modelling surface area and particle size effects, both the Ignition and Growth model and the Hot Spot model are inappropriate. The Ignition and Growth model was not specifically designed to model particle size effects. These can be included, using the method of Cochran and Tarver [30], but by then the number of

adjustable constants becomes unwieldy, and are too numerous to be experimentally determined at MRL. The Hot Spot model has been used successfully to simulate particle size effects [34], but the process is not straightforward, and requires a high degree of familiarity with the model. Both the DAGMAR and Krakatoa models are also inappropriate, as neither addresses the problem of particle size effects. The multiphase models briefly discussed in Section 6 must also be ruled out because we currently do not have the multiphase code capability to implement them.

The most promising approach is the Kim model. This has the advantage of having been specifically formulated to model particle size effects, as well as requiring the experimental determination of only a small number of adjustable constants. It also uses the HOM equation of state for both reactants and products, which is the equation of state used by both the SIN and 2DL codes. The disadvantage with this model, as previously noted, is that the heat conduction equation has to be solved within the shell of material surrounding the hollow sphere within each hydrodynamic cell for each hydrodynamic time step. This is not a trivial consideration, and makes the implementation of the model into an existing hydrocode far from straightforward [31].

At MRL, the Kim model could currently be implemented into the 1D Lagrangian finite difference code SIN. This code has the advantage of being well documented [4], but has the disadvantage that it uses the artificial viscosity method to handle shock formation [43]. This successfully dampens oscillations around the shock front, but can also lead to problems when parameters reflecting real viscosity effects need to be fitted to experimental data. Models of hot spot formation based on viscoplastic heating are a case in point, and problems of this type have already been encountered with the Kim model [31] during its current implementation in a 1D finite difference Lagrangian code known as STEALTH [23], which also uses the artificial viscosity method for shock formation.

These problems could be overcome by implementing the Kim model in a 1D Flux Corrected Transport (FCT) code which is currently being designed at MRL [44]. FCT algorithms require no artificial viscosity terms and the shock front can be infinitely sharp. This would make identification of an accurate value for the material viscosity in the Kim model much easier.

Most hydrocodes used by the explosives community to date use the artificial viscosity method to handle shock formation. However, there have been many improvements in recent years in the numerical schemes developed for solving the equations of ideal compressible flows, and none of these techniques requires the use of an artificial viscosity term. The explosives community has, in general, been slow to adapt these newer methods to the more complex reacting flows. One exception is the work of Oran, Boris and their collaborators [48]. They have used the finer shock resolution available with FCT algorithms to gain valuable insights into the stability of detonation in gaseous and liquid explosives. Two papers in the coming Ninth Symposium (International) on Detonation [49,50] also show the gradual adoption of these newer techniques. One of the advantages of these newer methods is that the finer shock resolution allows a more accurate determination of the radius of curvature of a two dimensional detonation front. Recent theories connecting curvature with reaction rate then allow information to be obtained on the rate of energy release within the explosive [50,51]. Information of this type is currently of interest to MRL for some recent PBX formulations.

In conclusion, the Kim model should be used to simulate particle size effects, and the model should be implemented in either the SIN hydrocode, or an FCT hydrocode currently under development at MRL. The FCT hydrocode is preferred, for reasons discussed above, but implementation in either hydrocode will not be straightforward.

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Table 1 Values of constants for original Ignition and Growth model [7].

EXPLOSIVE	PBX-9404	TATB	PETN	CAST TNT
I (Is)	44	50	20	50
G (Is Mbars^{-Z})	200	125	400	40
Z	1.6	2.0	1.4	1.2

Table 2 Values of constants for modified Ignition and Growth model [8].

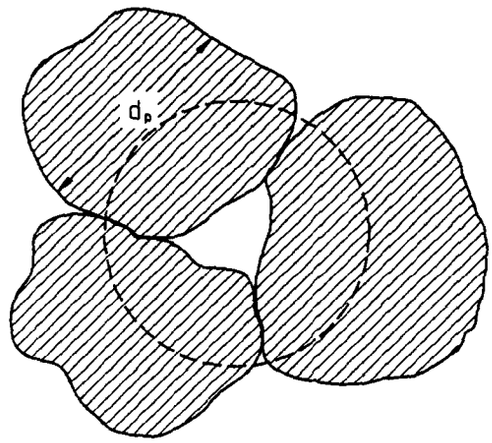
EXPLOSIVE	PBX-9404	LX-17
I (Is)	7.43×10^{11}	4.0×10^{6}
b	0.667	0.667
a	0.0	0.22
x	20.0	7.0
G_1 (Mbars^{-y} Is)	3.1	0.6
c	0.667	0.667
d	0.111	0.111
y	1.0	1.0
G_2 (Mbars^{-z} Is)	400.0	400.0
e	0.333	0.333
g	1.0	1.0
z	2.0	3.0

TABLE OF SYMBOLS

F	Fraction of reacted explosive (Ignition and Growth model)
ρ	Density. ρ_o is initial density, ρ_s is density of shocked explosive.
η	$\rho_s/\rho_o - 1$
I, G, r, x, y, z	Constants in the Ignition and Growth model which must be determined by fitting to experiment.
G_1, G_2, a, b, c, d, e, g	Constants in the modified Ignition and Growth model which must be determined by fitting to experiment.
ϵ	Strain
σ	Stress. σ_o is the static yield strength, σ_r radial stress, σ_θ tangential stress.
γ_1	Coefficient of viscosity
E	Young's modulus
r	Radial space coordinate
v	Radial velocity
γ	$\gamma_1\sigma_o$
k	$\sigma_o/\sqrt{3}$
k^*	Thermal conductivity
r_i, r_o	Inner and outer radii of hollow sphere used in Kibong Kim model.
P	Pressure. P_o is applied stress at r_o, P_g is gas pressure in the void.
C_p	Heat capacity at constant pressure.
Q	Heat of reaction
T	Temperature. T^* is an activation temperature.
λ	Reaction rate variable
Z	Frequency factor in Arrhenius reaction rate.
τ_s	Characteristic time for hot spot excitation.
τ_c	Characteristic time for hot spot decomposition

TABLE OF SYMBOLS
(continued)

τ_m	Characteristic time for transport of energy from hot spots to colder bulk explosive.
τ_d	Characteristic time for decomposition of bulk explosive.
μ	Hot spot mass fraction
f_o	Threshold value of the normalized hot spot mass fraction.
λ_h	Mass fraction of hot spot products divided by μ.
λ_b	Mass fraction of the products of the balance of the explosive divided by $(1 - \mu)$.
P_s	Shock strength
m	Constant in Arrhenius expression
N_o	Number of hot spots per unit volume
ϕ_i	Volume fraction of phase i
C_i^+	Mass transfer rate for phase i

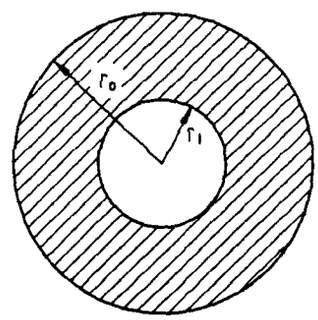


Average Particle Diameter = d_p

Porosity = 2%

$d_p \approx 200\mu m$

(a) Typical void in porous explosive.



$r_o \approx 100\mu m$

$r_i = (0.02)^{1/3} r_o$

(b) Idealization in Hollow Sphere Model.

Figure 1 The Hollow Sphere Model

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ABSTRACT

Several recent models for the shock initiation of heterogeneous explosives are presented, concentrating on those models which have proved to be the most successful. Particular attention is given to models of specific interest to MRL, which are capable of simulating the effect of particle size on sensitivity, and can be readily incorporated into single phase hydrodynamic computer codes. Other models are also briefly considered. Recommendations are made regarding the suitability of some of these models for MRL use.